

What is claimed is:

1. A crystallized Estrogen Receptor- β (ER- β) complexed with genistein.
2. The crystallized complex of Claim 1, characterized as having space group $P2_12_12_1$, and unit cell parameters of $a=53.49\text{\AA}$, $b=85.21\text{\AA}$, and $c=107.07\text{\AA}$.
3. An active site of a genistein binding protein or peptide, wherein said active site comprises the relative structural coordinates of amino acid residues MET343, LEU346, LEU349, GLU353, MET384, LEU387, MET388, ARG394, PHE404, ILE421, ILE424, GLY520, HIS523 and LEU524 according to Figure 2 for monomer A of ER- β , \pm a root mean square deviation from the backbone atoms of said amino acids of not more than 1.5\AA .
4. The active site of Claim 3, wherein the structural coordinates further comprises the relative structural coordinates of amino acid residues VAL328, MET342, SER345, THR347, LYS348, LEU349, ALA350, ASP351, LEU354, MET357, TRP383, GLU385, VAL386, MET389, GLY390, LEU391, MET392, LEU402, ILE403, ALA405, LEU408, VAL418, GLU419, GLY420, LEU422, GLU423, PHE425, LEU428, ALA516, SER517, LYS519, MET521, GLU522, LEU525, ASN526, MET527, LYS528, VAL533, VAL535, TYR536 and LEU538 according to Figure 2 for monomer A of ER- β , \pm a root mean square deviation from the backbone atoms of said amino acids of not more than 1.5\AA .
5. An active site of a genistein binding protein or peptide, wherein said active site comprises the relative structural coordinates of amino acid residues MET343, LEU346, LEU349, GLU353, MET384, LEU387, MET388, LEU391, ARG394, PHE404, ILE421, ILE424, GLY520, HIS523 and LEU524

according to Figure 2 for monomer B of ER- β , \pm a root mean square deviation from the backbone atoms of said amino acids of not more than 1.5Å.

6. The active site of Claim 4, wherein the structural coordinates further comprises the relative structural coordinates of amino acid residues MET342, SER345, THR347, LYS348, ALA350, ASP351, MET357, TRP383, GLU385, VAL386, LEU387, MET389, GLY390, MET392, LEU402, ILE403, ALA405, LEU408, VAL418, GLU419, GLY420, LEU422, GLU423, PHE425, LEU428, ALA516, SER517, LYS519, MET521, GLU522, LEU525, ASN526, MET527, LYS528, VAL533, TYR536 and LEU538 according to Figure 2 for monomer B of ER- β , \pm a root mean square deviation from the backbone atoms of said amino acids of not more than 1.5Å.

7. A method for identifying an agent that interacts with ER- β , comprising the steps of:

(a) generating a three dimensional model of ER- β using the relative structural coordinates according to Figure 2, \pm a root mean square deviation from the backbone atoms of said amino acids of not more than 1.5Å; and

(b) employing said three-dimensional model to design or select an agent that interacts with ER- β .

8. The method of Claim 7, further comprising the steps of: (c) obtaining the identified agent; and (d) contacting the identified agent with ER- β in order to determine the effect the agent has on ER- β activity.

9. A method for identifying an activator or inhibitor of a molecule or molecular complex comprising a genistein binding site, comprising the steps of:

(a) generating a three dimensional model of said molecule or molecular complex comprising a genistein binding site using (i) the relative structural coordinates of amino acid residues MET343, LEU346, LEU349,

GLU353, MET384, LEU387, MET388, ARG394, PHE404, ILE421, ILE424, GLY520, HIS523 and LEU524 according to Figure 2 for monomer A of ER- β , \pm a root mean square deviation from the backbone atoms of said amino acids of not more than 1.5Å, or (ii) the relative structural coordinates of amino acid residues MET343, LEU346, LEU349, GLU353, MET384, LEU387, MET388, LEU391, ARG394, PHE404, ILE421, ILE424, GLY520, HIS523 and LEU524 according to Figure 2 for monomer B of ER- β , \pm a root mean square deviation from the backbone atoms of said amino acids of not more than 1.5Å; and

(b) selecting or designing a candidate activator or inhibitor by performing computer fitting analysis of the candidate activator or inhibitor with the three dimensional model generated in step (a).

10. The method of Claim 9, wherein the structural coordinates according to (i) further comprises the relative structural coordinates of amino acid residues VAL328, MET342, SER345, THR347, LYS348, LEU349, ALA350, ASP351, LEU354, MET357, TRP383, GLU385, VAL386, MET389, GLY390, LEU391, MET392, LEU402, ILE403, ALA405, LEU408, VAL418, GLU419, GLY420, LEU422, GLU423, PHE425, LEU428, ALA516, SER517, LYS519, MET521, GLU522, LEU525, ASN526, MET527, LYS528, VAL533, VAL535, TYR536 and LEU538 according to Figure 2 for monomer A of ER- β , \pm a root mean square deviation from the backbone atoms of said amino acids of not more than 1.5Å.

11. The method of Claim 9, wherein the relative structural coordinates according to (ii) further comprises the relative structural coordinates of amino acid residues MET342, SER345, THR347, LYS348, ALA350, ASP351, MET357, TRP383, GLU385, VAL386, LEU387, MET389, GLY390, MET392, LEU402, ILE403, ALA405, LEU408, VAL418, GLU419, GLY420, LEU422, GLU423, PHE425, LEU428, ALA516, SER517, LYS519, MET521, GLU522, LEU525, ASN526, MET527, LYS528, VAL533, TYR536 and LEU538 according to Figure 2

for monomer B of ER- β , \pm a root mean square deviation from the backbone atoms of said amino acids of not more than 1.5Å.

12. The method of Claim 9, which further comprises the steps of: (c) obtaining the candidate activator or inhibitor; and (d) contacting the candidate activator or inhibitor with the molecule or molecular complex and determining the effect the candidate activator or inhibitor has on the molecule or molecular complex.

13. The method of Claim 12, wherein the candidate activator or inhibitor is contacted with the molecule or molecule complex in the presence of genistein in order to determine the effect the candidate activator or inhibitor has on binding of the molecule or molecular complex to genistein.

14. An agent identified by the method of Claim 7.

15. An inhibitor or activator identified by the method of Claim 9.